Thermal and Mechanical Properties of some FCC Transition Metals and their Binary Alloys

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(February 1, 2008)

Abstract

The temperature dependence of thermodynamic and mechanical properties of six fcc transition metals (Ni, Cu, Ag, Au, Pt, Rh) and the alloying behavior of Ag-Au and Cu-Ni are studied using molecular dynamics (MD). The structures are described at elevated temperatures by the force fields developed by Sutton and co-workers within the context of tight binding approach. MD algorithms are based on the extended Hamiltonian formalism from the works of Andersen, Parinello and Rahman, Nosé, Hoover and Çağın. The SIMULATOR program that we use generates information about various physical properties during the run time along with critical trajectory and stepwise information which need to be analyzed post production. The thermodynamic and mechanical properties are calculated in the temperature range between 300K to 1500K with 200K increments using the statistical fluctuation expressions over the MD trajectories.

65.70.+y, 61.66.Dk, 62.20.-x, 62.20.D, 67.40.Kh, 05.20.G

I. INTRODUCTION

The theoretical and computational modeling is becoming increasingly important in the development of advanced high performance materials for industrial applications. Atomistic level understanding of the properties of fcc transition metals under various conditions is important in their technological applications. The behavior of pure silver, gold, copper, nickel, platinum, rhodium and their alloys are tested over a wide temperature range using the potentials developed by Sutton and co-workers[1,2] for simulation. Our computer simulation results for Pt-Rh alloys are presented in elsewhere[3]. The MD algorithms that we use are based on the extended Hamiltonian formalism and the ordinary experimental conditions are simulated using the constant-pressure, constant-temperature (NPT) MD method.

Computer simulations on various model systems usually use simple pair potentials. On many occasions to account for the directionality of bonding, three body interactions are also employed. The interactions in real crystalline materials can not be represented by simple pairwise interactions alone. Pure pairwise potential model gives the Cauchy relation between the elastic constants $C_{12} = C_{44}$,which is not the case in real metals. In these systems the electron density plays a dominant role in interactions and resulting physical properties. Therefore, many-body interactions should be taken into consideration in any study of metals and metal alloys. In simple sp-bonded metals, the interaction potentials may be derived from model pseudopotentials using the second order perturbation theory. We have developed interaction potentials along these lines, and utilized them to study the properties of simple alkali metal and alkali metal alloys in the past[4]. However, for d-band metal and metal alloys the model pseudopotential approach should give way to newer techniques evolved over the past ten years to account for the many body effects. Among these approaches, the empirical many body potentials based on Norskov's Effective Medium Theory[5], Daw and Baskes' Embedded Atom Method[6], Finnis and Sinclair's[7,8] empirical many body potentials, and more recently the many body potentials developed by Sutton and co-workers[1,2] within the context of tight binding approach[9] for fcc transition metals can

be listed. Due to its mathematically simple power law form and fairly long range character, in recent years the Sutton-Chen (SC) potential has been widely used in simulations to study a range of problems[10–16].

II. THE METHOD

In the SC description the total potential energy of the metal is given as a sum of a pairwise repulsion term and a many-body density dependent cohesion term. The cohesion term supplies the description of short-range interactions to obtain a good description of surface relaxation, and the pairwise term gives a correct description of long-range interactions with a van der Waals tail. The functional form of the interaction potential is as follows:

$$U_i = D\left(\frac{1}{2}\sum_j u(\mathbf{r_{ij}}) - c\rho_i\right) \quad , \tag{1}$$

where

$$u(r) = (\frac{a}{r})^n \quad , \tag{2}$$

$$\rho_i = \left(\sum_j \phi(r_{ij})\right)^{\frac{1}{2}} \quad , \tag{3}$$

$$\phi(r) = \left(\frac{a}{r}\right)^m \quad . \tag{4}$$

The Sutton-Chen potential parameters D, c and m and n are optimized to fit to the 0 K properties such as the cohesive energy, zero pressure condition and the bulk modulus of the f.c.c. metals. In Table:1, the values of these parameters for Ni, Cu, Ag, Au, Pt and Rh are listed.

The functional form of the Sutton-Chen potential is fairly simple in comparison to Embedded Atom Method potentials and is moderately long ranged. The last property makes this set especially attractive for surface and interface studies amongst others, since most of them are very short ranged (are fitted up to first or second nearest neighbor distances).These interaction potentials can be generalized to describe binary metal alloys in such a way that all the parameters in the Hamiltonian equations are obtained from the parameters of pure

metals. The Sutton-Chen interaction potential above is adopted by Rafii-Tabar and Sutton[2] to a random f.c.c. alloy model in which sites are occupied by two types of atoms completely randomly, such that the alloy has the required average concentration. The equilibrium lattice parameter a^* at 0 K of the random alloy is chosen as the universal length scale and the expectation value E^t per atom of the interaction Hamiltonian is given as a function of a^*. Rafii-Tabar and Sutton after determining the value of the equilibrium lattice parameter for the random alloy, they calculated elastic constants and enthalpy of mixing by *static* lattice summation method. Once a^* is found the enthalpy of mixing ΔH per atom at 0 K are also obtained from

$$\Delta H = E^t - c_A E^A - c_B E^B \quad , \tag{5}$$

where E^A and E^B are the cohesive energies per atom of the elemental A and B metals and the constants are such that $c_A + c_B = 1$.

In this paper we aim at using the Molecular Dynamics method to obtain the a^* and the enthalpy of mixing per atom for alloys. In the following the expressions specific to many body potentials which are used in our computations are presented.The many body force on atom a along a direction $i(= x, y, z)$ is given as:

$$F_{ia} = -\frac{D}{2}\left(\sum_b^* u'(r)\frac{r_{abi}}{r_{ab}} - \frac{c_a}{2}\frac{\sum_b^* \phi'(r)\frac{r_{abi}}{r_{ab}}}{\rho_a}\right), \tag{6}$$

where $'$ denotes $\frac{\partial}{\partial r}$ and * signifies the exclusion of $a = b$ from the sums. The anisotropic stress tensor including the contribution from the many body potential is calculated from

$$\Omega P_{ij} = \sum_a \frac{p_{ai}p_{aj}}{m_a} - \frac{D}{2}\sum_a\left(\sum_b^* u'(r)\frac{r_{abi}r_{abj}}{r_{ab}} - \frac{c_a}{2}\frac{\sum_b^* \phi'(r)\frac{r_{abi}r_{abj}}{r_{ab}}}{\rho_a}\right), \tag{7}$$

The potential energy contribution to the elastic constants, the hypervirial tensor χ_{ijkl}, is given as

$$\begin{aligned}\Omega\chi_{ijkl} = \frac{D}{2}\sum_a(\sum_b^*(u'' - \frac{u'}{r_{ab}})\frac{r_{abi}r_{abj}r_{abk}r_{abl}}{r_{ab}^2} \\ -\frac{c_a}{2}\frac{\sum_b^*(\phi'' - \frac{\phi'}{r_{ab}})\frac{r_{abi}r_{abj}r_{abk}r_{abl}}{r_{ab}^2}}{\rho_i} \\ +\frac{c_a}{4}\frac{(\sum_b^*\phi'\frac{r_{abi}r_{abj}}{r_{ab}})(\sum_c^*\phi'\frac{r_{ack}r_{acl}}{r_{ac}})}{\rho_a^3}).\end{aligned} \tag{8}$$

In our computations at each concentration and at each temperature, first the zero strain state ,h_o, of the system is determined by performing constant temperature and constant stress simulations (NPT)at zero stress. This yields the reference shape and size matrix, h_o in Parrinello-Rahman formalism. In determining elastic constants this reference state is used in constant temperature constant volume simulations (NVE) of 50000 steps for each state point. The elastic constants are evaluated using the following statistical fluctuation formulas[17]

$$C^T_{ijkl} = -\frac{\Omega_o}{k_B T}(< P_{ij}P_{kl} > - < P_{ij} >< P_{kl} >) + \frac{2Nk_BT(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk})}{\Omega_o} + < \chi_{ijkl} > \quad (9)$$

where <> denotes the averaging over time and $\Omega_o = deth_o$ is the reference volume for the model system. The first term represents the contribution from the fluctuation of the microscopic stress tensor, P_{ij}, the second term represents the kinetic energy contribution, and the third term is the Born term.

We use the program **Simulator** developed by Çağın that employs the state of the art MD algorithms based on extended Hamiltonian formalisms emerging from the works of Anderson[18], Parinello and Rahman[19], Nosé[20], Hoover[21] and Çağın[22]. A 500 atoms cubical system is used and the simulation started with atoms randomly distributed on a fcc lattice.The system is thermalized starting from 1K to the target temperature using a constant enthalpy and constant pressure (NHP) ensemble by slowly heating while scaling velocities to increment the temperature of 1K/step over the specific number of steps depending on the target temperature. This is followed by strict velocity scaling at each target temperature. Then, NPT dynamics at this temperature for 20000 steps to calculate the volume, density and enthalpy of the system for each concentration is performed. The resulting zero strain averaged matrix $< h_0 >$ is used in calculating elastic constants over 50000 steps of NVE dynamics. A fifth-order Gear predictor-corrector algorithm is used in Δt = 2 fs.The Parrinello-Rahman piston mass parameter is chosen as W=400 and in NPT runs the Nosé-

Hoover parameter is set to Q=100.

III. RESULTS AND DISCUSSION

In this section,the molecular simulation results obtained for pure f.c.c. transition metals, Ni, Cu, Ag, Au, Pt and Rh are presented. In Tables 2 to 7, the results of NPT molecular dynamics simulations of pure elements after 20000 steps are shown. These are density, enthalpy, potential energy and volume of 500 atoms calculated at different temperatures. In obtaining these values the system is thermalized starting from 1K to the target temperature using 20000 steps NHP simulations. We then performed another 20000 steps NPT dynamics at the target temperature. In order to show the behavior of Sutton-Chen potentials at elevated temperatures; the results of density and enthalpy are plotted at temperatures 300K, 500K, 750K and 1000K in Figures 1 and 2. The extra datas for Pt and Rh at temperatures 700K, 900K, 1100K, 1300K and 1500K are coming from the calculations of Pt-Rh alloys[3]. In Tables 2 to 7 at 300K, the experimental and simulation results of the densities are shown. Simulation results show approximately 2.0% deviation from the experimental values for Ni,Cu,Ag,Au and 1.4% and 1.0% for Pt and Rh respectively. The percent change in the lattice parameter at each temperature (the lattice parameter at 300K is used as the reference) for Ni, Cu , Ag, Au are given in Table 8, Pt and Rh results are being discussed in[3]. As a concluding remark, it can be said that as the temperature increases the deviation from the experimental values increases.

In Tables 9 to 14 , the results of the calculations of the elastic constants and bulk moduli of Ni, Cu, Ag, Au, Pt and Rh obtained from NVE simulations of 50000 steps are presented. Elastic constants are calculated in the temperature range between 300K to 1000K. In the calculations at each concentration and at each temperature first the zero-strain state of the system is determined by performing constant-temperature and constant-stress simulations. In determining the elastic constants this reference state is used in constant-temperature, constant-volume simulations of 50000 steps for each state point. Comparison

with experimental results is possible only at 100K and this is shown in Table 15. The ratio of C_{12}/C_{44} is 2.38 for Ni, 2.42 for Cu, 1.75 for Ag, 3.76 for Au, 3.68 for Ph and 1.69 for Rh. Figures 3 to 8 show the variations of elastic constants of Ni, Cu, Ag, Au, Pt, Rh with respect to temperature. The change in the bulk moduli of these metals by heating is shown in Figure 9 . The simulation values of the bulk moduli at 1000K are the fingerprints for the melting temperature of these metals. The bulk modulus is higher for higher melting temperature. The elastic constants results show that the crystals are elastically stable since the stability conditions $C_{44} > 0$, $C_{11} > 0$ and $C_{11} > C_{12}$ are satisfied and thermal softening behavior is observed as the temperature is increased.

In Tables 16 and 17, the simulation results of Ag-Au and Cu-Ni binary alloys are given. These are the enthalpy of mixing and the densities of Ag-Au and Cu-Ni alloys at 300K. In Figure 10, the densities of Cu-Ni and Ag-Au are drawn with respect to atomic concentrations. Again in Figure 11, the enthalpy of mixing for the same alloys are drawn as a function of atomic concentrations. The sign of enthalpy of mixing is correct at all concentration values. The mixing of these alloys are enthalpically favorable. The potentials used in the present dynamic simulations give reasonably accurate description of the thermodynamic properties and the elastic constants. Altough, the parametrization of these potentials are based on the bulk properties at 0K, still it can describe the temperature-dependent behavior of the solid correctly. We find that with an improved parameter sets the Sutton-Chen potential does quite well in predicting a number of properties of fcc metals in MD simulations. In order to simulate the ordinary experimental conditions (constant pressure) the NPT MD method works quite well and determining the zero strain state, h_o, of the system at each concentration and at each temperature is curicial in simulations.

ACKNOWLEDGMENTS

This research is supported by the Scientific and Technical Research Council of Turkey (TUBITAK) through the Project TBAG 1592 and by the Middle East Technical University

Research Fund through the Project AFP-96-01-05-03.

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FIGURES

TABLES

TABLE I. Sutton-Chen potential parameters for f.c.c. metals.

a ($\AA$)	D ($10^{-2}eV$)	c	m	n	Metal
3.52	1.57070	39.432	6	9	Ni
3.61	1.23820	39.432	6	9	Cu
4.09	0.25415	144.410	6	12	Ag
4.08	1.27930	34.408	8	10	Au
3.92	1.98330	34.408	8	10	Pt
3.80	0.49371	144.410	6	12	Rh

TABLE II. The density, enthalpy, potential energy and volume of Ni as obtained from NPT molecular dynamics simulations after 20000 steps. The number in parenthesis is the corresponding experimental value at that temperature.

T (K)	ρ (g/cm^3)	H (kJ/mol)	U (kJ/mol)	500 x V_0 (nm^3)
300	8.7468 (8.90)	-420.77492	-424.51844	5.571
500	8.6327	-415.54424	-421.78116	5.645
750	8.4815	-408.77260	-418.12898	5.745
1000	8.3176	-401.66660	-414.13714	5.858

TABLE III. The density, enthalpy, potential energy and volume of Cu as obtained from NPT molecular dynamics simulations after 20000 steps. The number in parenthesis is the corresponding experimental value at that temperature.

T (K)	ρ (g/cm^3)	H (kJ/mol)	U (kJ/mol)	500 x V_0 (nm^3)
300	8.7235 (8.912)	-330.03778	-333.77963	6.048
500	8.5742	-324.71396	-330.95169	6.153
750	8.3717	-317.73297	-327.08560	6.302
1000	8.1334	-310.01874	-322.48972	6.486

TABLE IV. The density, enthalpy, potential energy and volume of Ag as obtained from NPT molecular dynamics simulations after 20000 steps. The number in parenthesis is the corresponding experimental value at that temperature.

T (K)	ρ (g/cm^3)	H (kJ/mol)	U (kJ/mol)	500 x V_0 (nm^3)
300	10.2710 (10.49)	-277.95578	-281.69931	8.719
500	10.1030	-272.64944	-278.88458	8.864
750	9.8755	-265.69861	-275.05511	9.068
1000	9.6191	-258.25937	-270.73138	9.310

TABLE V. The density, enthalpy, potential energy and volume of Au as obtained from NPT molecular dynamics simulations after 20000 steps. The number in parenthesis is the corresponding experimental value at that temperature.

T (K)	ρ (g/cm^3)	H (kJ/mol)	U (kJ/mol)	500 x V_0 (nm^3)
300	18.8411 (19.32)	-357.05188	-360.79401	8.679
500	18.5168	-351.69836	-357.93332	8.831
750	18.0595	-344.58054	-353.93341	9.055
1000	17.4804	-336.48160	-348.95288	9.355

TABLE VI. The density, enthalpy, potential energy and volume of Pt as obtained from NPT molecular dynamics simulations after 20000 steps. The number in parenthesis is the corresponding experimental value at that temperature.

T (K)	ρ (g/cm^3)	H (kJ/mol)	U (kJ/mol)	500 x V_0 (nm^3)
300	21.1954 (21.50)	-557.82990	-561.57330	7.641
500	20.9757	-552.62994	-558.86822	7.722
700	20.7427	-547.30029	-556.03040	7.808
750	20.6825	-545.93384	-555.28748	7.831
900	20.4961	-541.79657	-553.02002	7.902
1000	20.3664	-538.96735	-551.43976	7.952
1100	20.2303	-536.06519	-549.78400	8.006
1300	19.9378	-530.03790	-546.25262	8.123
1500	19.5992	-523.49762	-542.20453	8.264

TABLE VII. The density, enthalpy, potential energy and volume of Rh as obtained from NPT molecular dynamics simulations after 20000 steps. The number in parenthesis is the corresponding experimental value at that temperature.

T (K)	ρ (g/cm^3)	H (kJ/mol)	U (kJ/mol)	500 x V_0 (nm^3)
300	12.3152 (12.45)	-547.24719	-550.99084	6.937
500	12.2184	-542.09912	-548.33862	6.992
700	12.1191	-536.88055	-545.61493	7.049
750	12.0937	-535.56250	-544.91638	7.064
900	12.0162	-531.56805	-542.78949	7.110
1000	11.9637	-528.87659	-541.34656	7.141
1100	11.9099	-526.14417	-539.86707	7.173
1300	11.7990	-520.59625	-536.80499	7.241
1500	11.6838	-514.93768	-533.62976	7.312

TABLE VIII. The linear expansion of Ni, Cu, Ag, and Au as a function of temperature.

T (K)		500	750	1000
Ni	This Work	0.44	1.04	1.72
	Experiment	0.29	0.69	1.13
Cu	This Work	0.58	1.40	2.42
	Experiment	0.34	0.82	1.36
Ag	This Work	0.55	1.34	2.26
	Experiment	0.43	0.99	1.61
Au	This Work	0.58	1.44	2.60
	Experiment	0.31	0.70	1.14

TABLE IX. Elastic constants and bulk modulus of Ni calculated at 300 K, 500 K, 750 K and 1000 K as obtained from NVE Molecular Dynamics Simulation after 50000 steps.

T (K)	C_{11} (GPa)	C_{12} (GPa)	C_{44} (GPa)	B (GPa)
300	213.76 ±0.19	166.57 ±0.20	69.77 ±0.21	182.30 ±0.20
500	201.70 ±0.21	159.48 ±0.51	63.56 ±0.20	173.55 ±0.41
750	186.05 ±0.66	150.34 ±0.06	55.94 ±0.55	162.24 ±0.26
1000	169.14 ±1.99	141.08 ±0.87	48.29 ±0.28	150.43 ±1.24

TABLE X. Elastic constants and bulk modulus of Cu calculated at 300 K, 500 K, 750 K and 1000 K as obtained from NVE Molecular Dynamics Simulation after 50000 steps.

T (K)	C_{11} (GPa)	C_{12} (GPa)	C_{44} (GPa)	B (GPa)
300	153.06 ±0.42	119.45 ±0.16	49.35 ±0.27	130.65 ±0.25
500	140.87 ±0.19	112.78 ±0.24	43.46 ±0.40	122.14 ±0.23
750	126.46 ±1.06	104.43 ±0.32	36.37 ±1.39	111.77 ±0.57
1000	109.09 ±0.66	94.40 ±0.94	27.92 ±0.65	99.30 ±0.85

TABLE XI. Elastic constants and bulk modulus of Ag calculated at 300 K, 500 K, 750 K and 1000 K as obtained from NVE Molecular Dynamics Simulation after 50000 steps.

T (K)	C_{11} (GPa)	C_{12} (GPa)	C_{44} (GPa)	B (GPa)
300	126.95 ±0.23	88.49 ±0.11	50.50 ±0.08	101.31 ±0.15
500	117.46 ±0.27	83.45 ±0.13	45.50 ±0.28	94.79 ±0.17
750	104.16 ±0.58	76.79 ±0.72	37.75 ±0.33	85.91 ±0.68
1000	91.88 ±0.86	70.59 ±1.27	31.54 ±0.80	77.69 ±1.14

TABLE XII. Elastic constants and bulk modulus of Au calculated at 300 K, 500 K, 750 K and 1000 K as obtained from NVE Molecular Dynamics Simulation after 50000 steps.

T (K)	C_{11} (GPa)	C_{12} (GPa)	C_{44} (GPa)	B (GPa)
300	158.24 ±0.64	131.56 ±0.02	34.92 ±0.10	140.45 ±0.23
500	141.74 ±0.75	118.92 ±0.21	30.08 ±0.56	126.52 ±0.39
750	123.92 ±0.62	107.42 ±0.92	24.10 ±0.58	112.92 ±0.82
1000	95.43 ±0.86	84.78 ±0.16	16.78 ±0.81	88.33 ±0.39

TABLE XIII. Elastic constants and bulk modulus of Pt calculated from 300 K to 1500 K with 200 K increments as obtained from NVE Molecular Dynamics Simulation after 50000 steps.

T (K)	C_{11} (GPa)	C_{12} (GPa)	C_{44} (GPa)	B (GPa)
300	289.63 ±1.02	239.55 ±0.16	65.07 ±0.28	256.24 ±0.45
500	272.67 ±0.87	227.11 ±0.77	59.67 ±0.36	242.29 ±0.80
700	256.12 ±1.71	214.38 ±0.78	54.15 ±0.59	228.30 ±1.09
750	251.09 ±1.06	211.05 ±0.72	52.90 ±0.28	224.34 ±0.84
900	233.28 ±0.40	196.58 ±0.32	49.08 ±0.50	208.81 ±0.35
1000	227.47 ±2.66	193.46 ±0.81	45.50 ±0.50	204.80 ±1.43
1100	219.39 ±0.80	188.60 ±0.62	44.12 ±1.51	198.86 ±0.68
1300	200.63 ±2.39	174.16 ±0.51	38.78 ±0.55	182.98 ±1.14
1500	177.28 ±2.46	155.50 ±0.40	31.94 ±1.96	162.76 ±1.09

TABLE XIV. Elastic constants and bulk modulus of Rh calculated from 300 K to 1500 K with 200 K increments as obtained from NVE Molecular Dynamics Simulation after 50000 steps.

T (K)	C_{11} (GPa)	C_{12} (GPa)	C_{44} (GPa)	B (GPa)
300	322.30 ±0.66	223.02 ±0.90	131.95 ±0.69	256.11 ±0.82
500	312.03 ±0.69	216.89 ±0.44	124.72 ±0.15	248.60 ±0.52
700	298.92 ±0.77	210.23 ±0.78	117.44 ±0.14	239.79 ±0.78
750	295.14 ±0.88	207.72 ±0.73	116.27 ±1.27	236.86 ±0.78
900	286.44 ±0.62	203.55 ±0.69	110.80 ±0.97	231.17 ±0.67
1000	279.36 ±1.12	199.07 ±0.71	108.16 ±1.07	225.83 ±0.84
1100	274.83 ±1.49	197.32 ±0.20	104.07 ±0.10	223.15 ±0.63
1300	263.48 ±0.77	191.06 ±2.16	97.36 ±0.88	215.20 ±1.70
1500	249.59 ±0.12	184.75 ±1.18	91.29 ±1.32	206.36 ±0.83

TABLE XV. Elastic constants of fcc metals in units of GPa at 300K. At each entry, the first number gives the MD simulation result while the second number in round brackets is the experimental value.

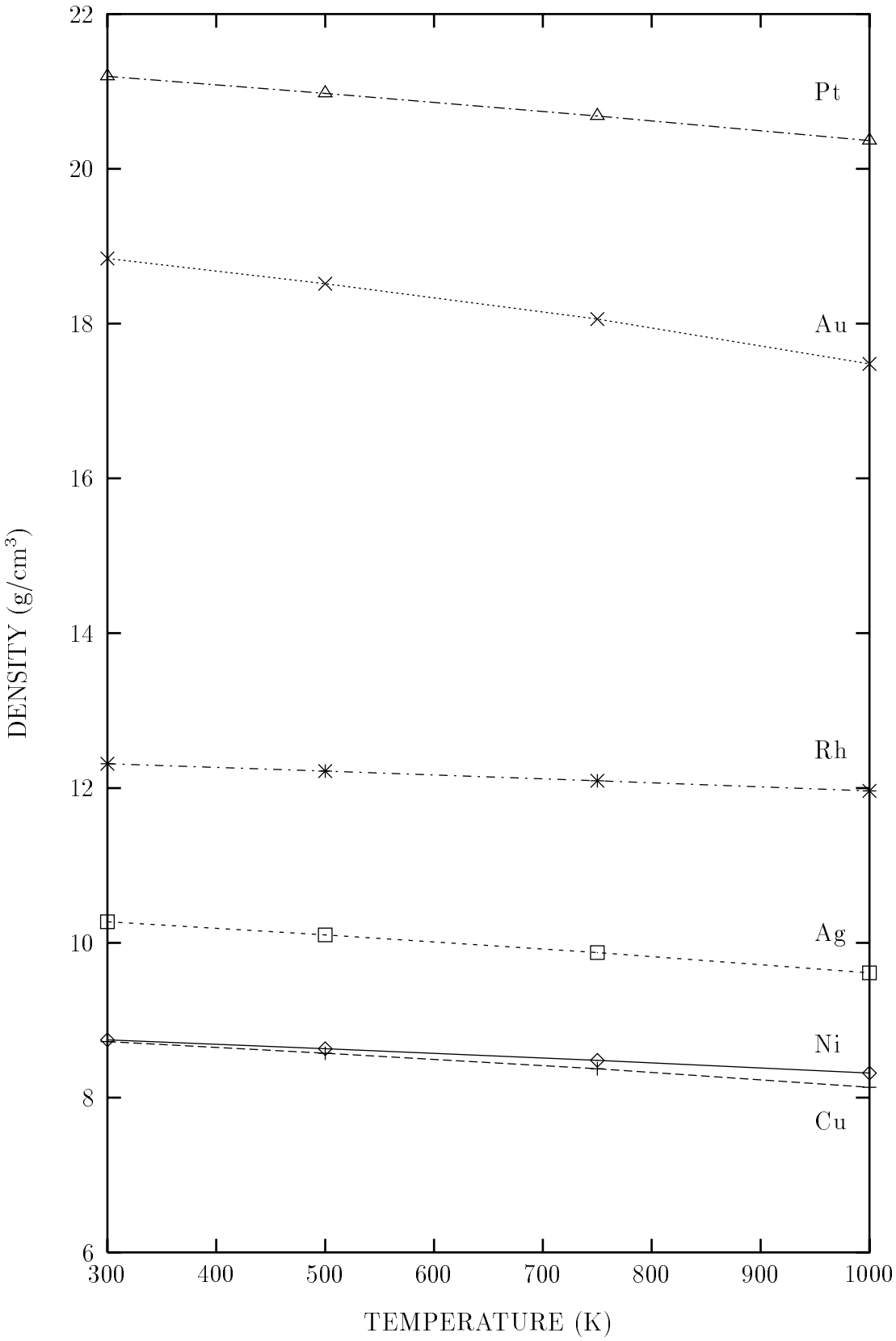
Metal	C_{11}	C_{12}	C_{44}
Ni	213.76 (250.8)	166.50 (150.0)	69.77 (123.5)
Cu	153.06 (168.39)	119.45 (121.42)	49.35 (75.39)
Ag	126.95 (123.99)	88.49 (93.67)	50.50 (46.12)
Au	158.24 (192.34)	131.56 (163.14)	34.92 (41.95)

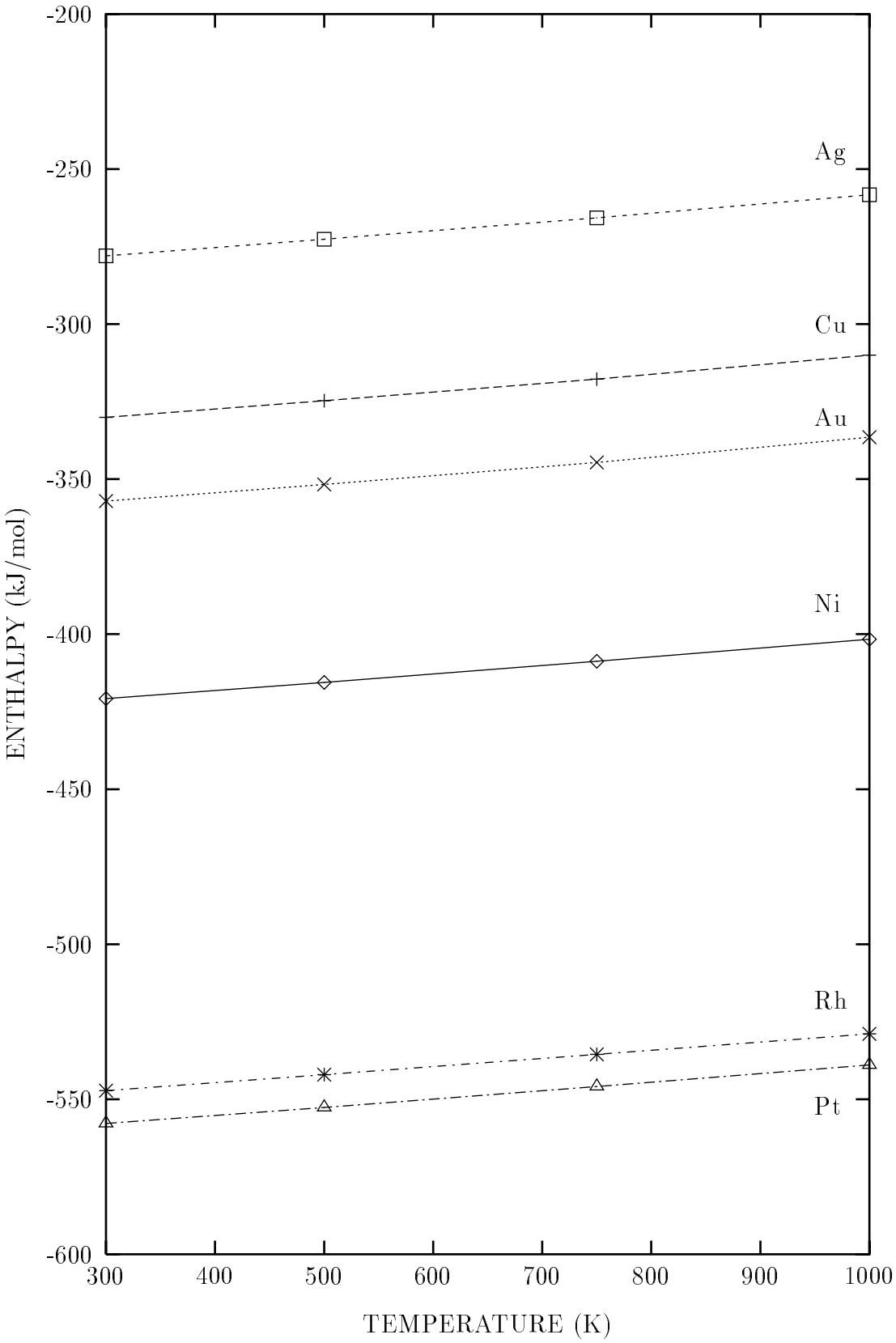
TABLE XVI. The enthalpy of mixing and density for the random Ag-Au binary alloy at T= 300 K as obtained from TPN molecular dynamics simulations after 20000 to 25000 steps.

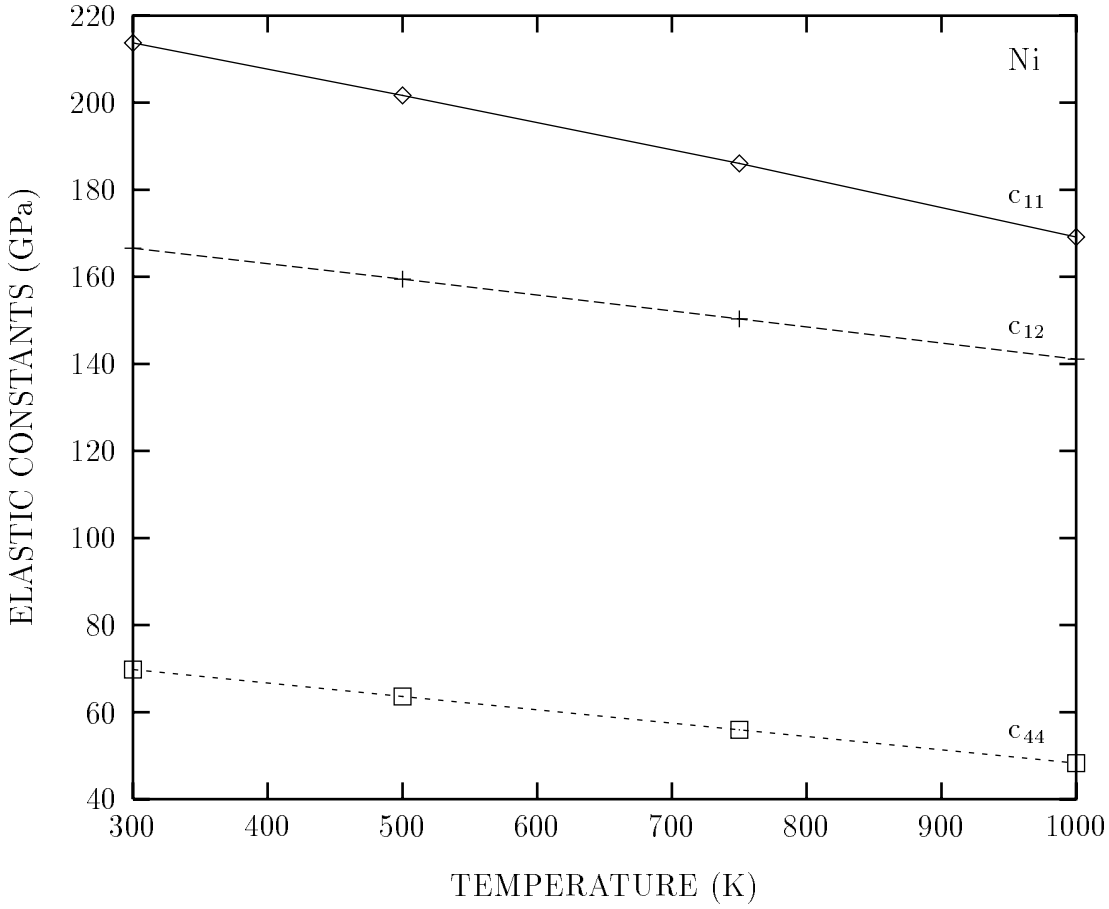
Percent Au @ Ag	ρ (g/cm^3)	H (kJ/mol)	Δ H (J/mol)
0	10.2708	-277.95450	0.0
10	11.1411	-286.73332	-869.67
20	12.0089	-295.38254	-1609.74
30	12.8757	-303.84702	-2165.07
40	13.7408	-312.16146	-2570.36
50	14.6009	-320.20978	-2709.53
60	15.4590	-328.08450	-2675.10
70	16.3107	-335.64754	-2328.99
80	17.1593	-343.42174	-2193.44
90	18.0029	-350.15168	-1014.83
100	18.8409	-357.04600	0.0

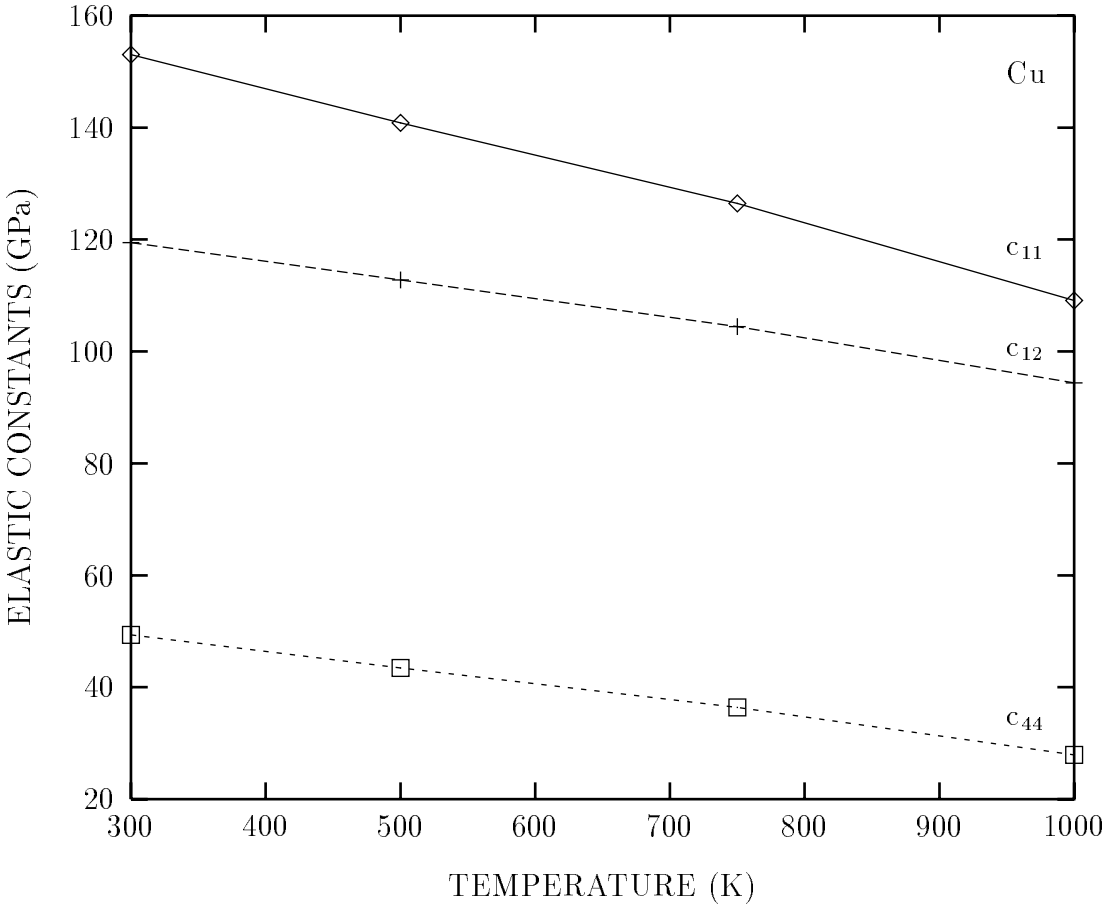
TABLE XVII. The enthalpy of mixing and density for the random Cu-Ni binary alloy at T= 300 K as obtained from TPN molecular dynamics simulations after 20000 to 25000 steps.

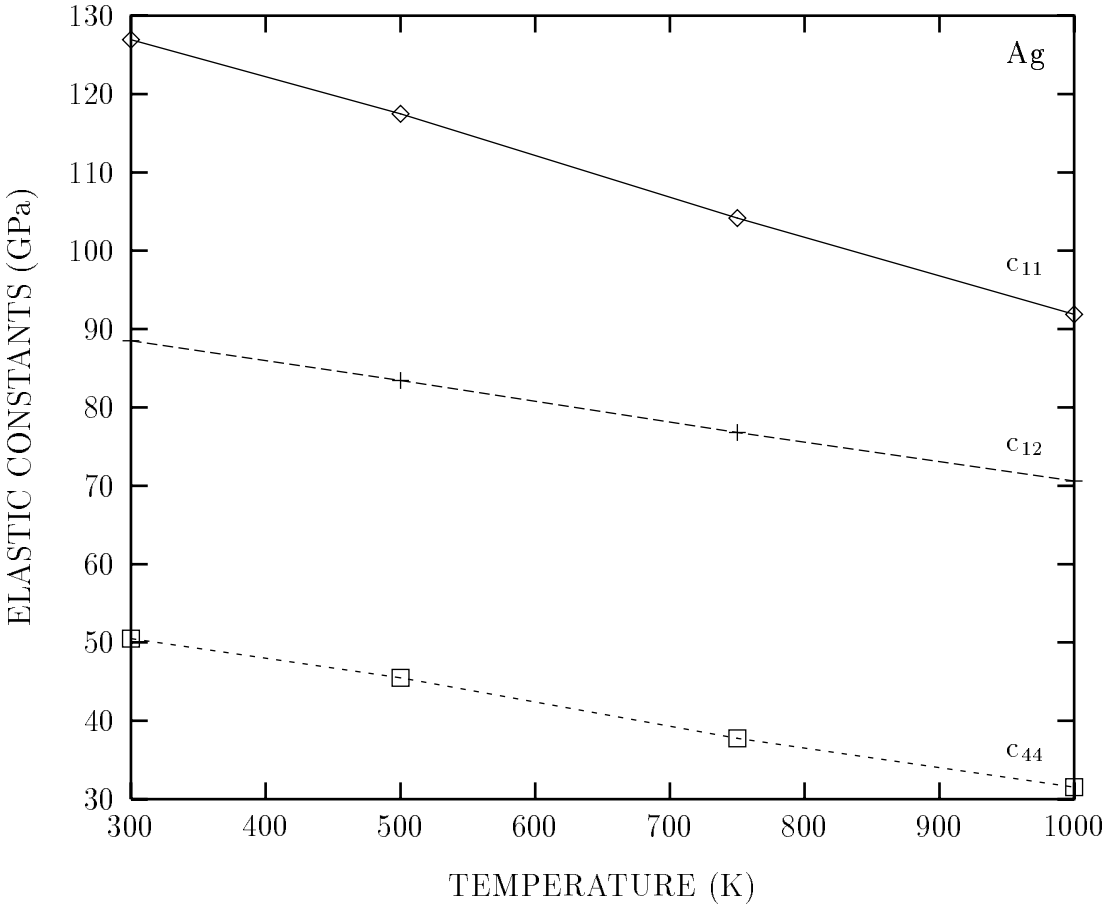
Percent Ni @ Cu	ρ (g/cm^3)	H (kJ/mol)	Δ H (J/mol)
0	8.7241	-330.03506	0.0
10	8.7368	-339.24688	-137.13
20	8.7490	-348.45416	-269.72
30	8.7560	-357.59454	-335.41
40	8.7629	-366.73834	-410.14
50	8.7667	-375.82918	-410.67
60	8.7663	-384.89876	-416.70
70	8.7650	-393.93110	-374.56
80	8.7611	-402.92374	-291.16
90	8.7550	-411.86898	-161.71
100	8.7691	-420.78196	0.0

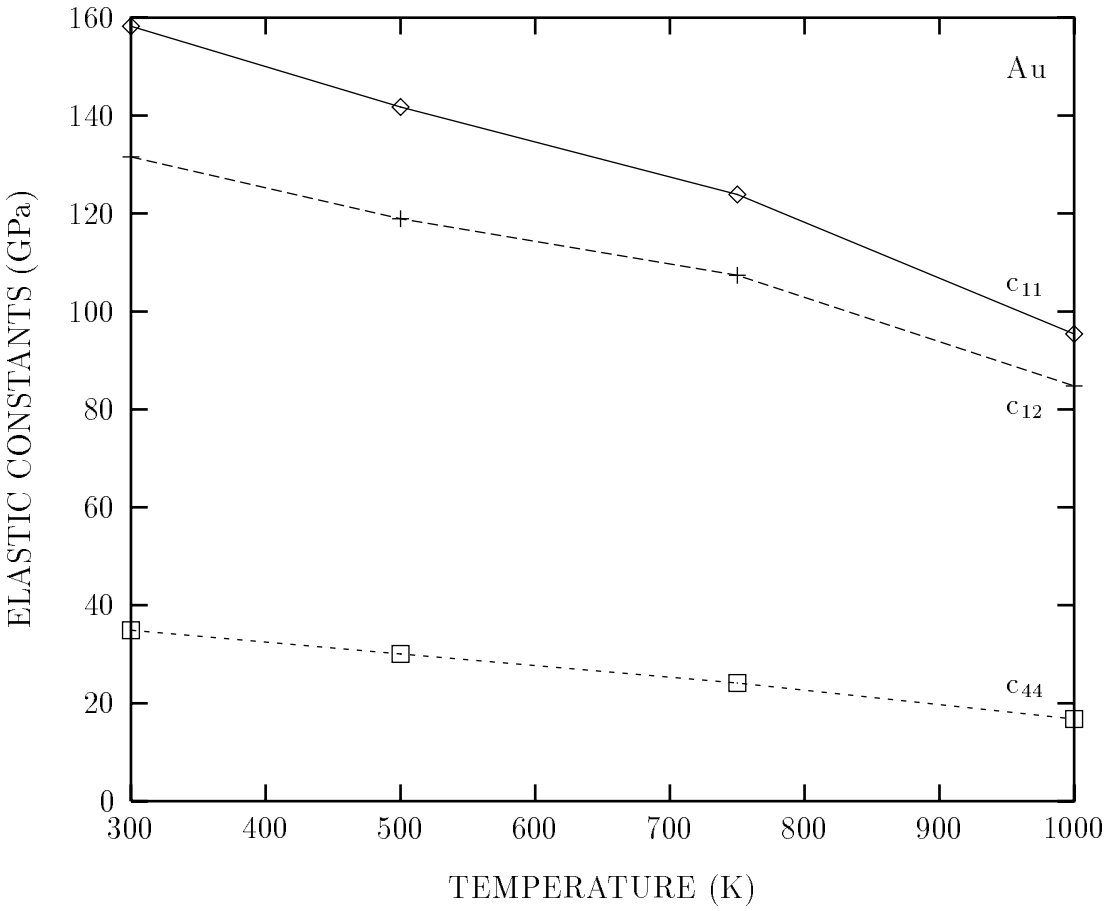

22
20
18
16
14
12
10
8
6
300
400
500
600
700
800
900
1000
DENSITY (g/cm^3)
TEMPERATURE (K)
Pt
Au
Rh
Ag
Ni
Cu

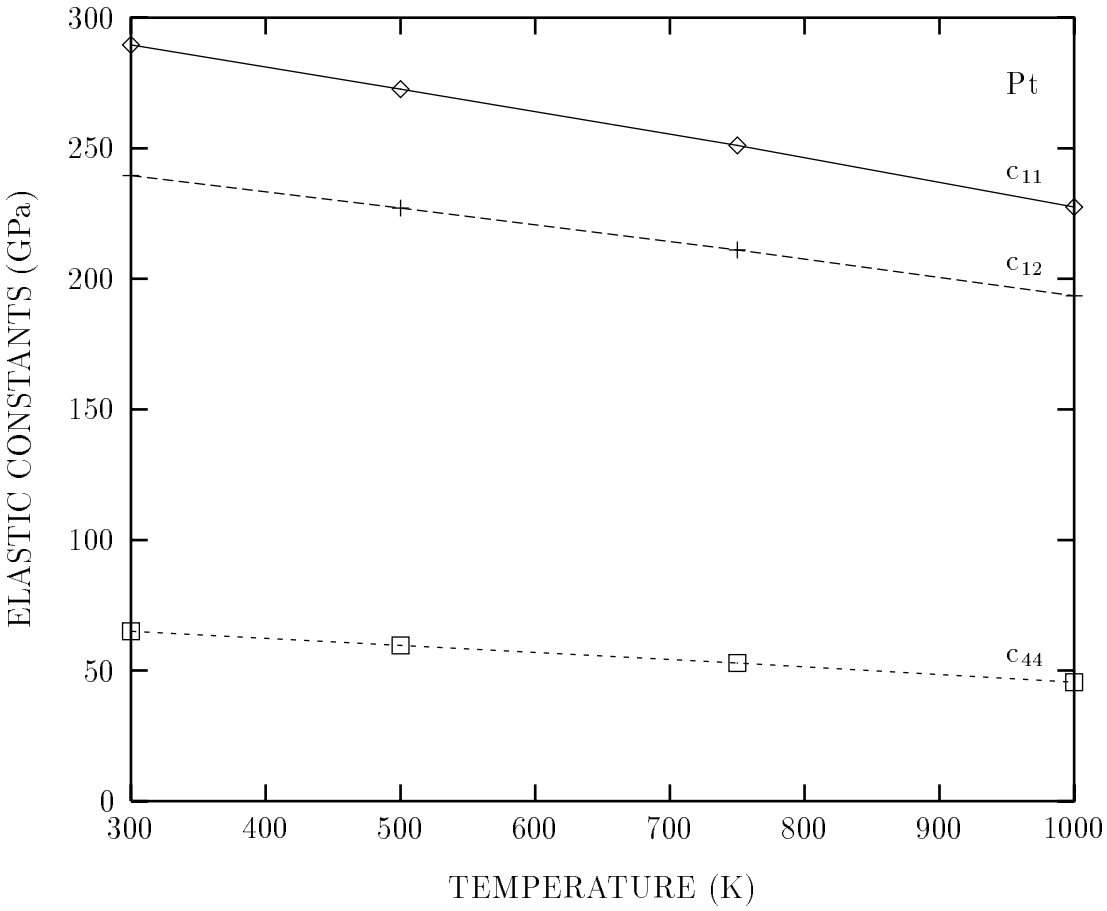

-200
-250
-300
-350
-400
-450
-500
-550
-600
ENTHALPY (kJ/mol)
300
400
500
600
700
800
900
1000
TEMPERATURE (K)
Ag
Cu
Au
Ni
Rh
Pt

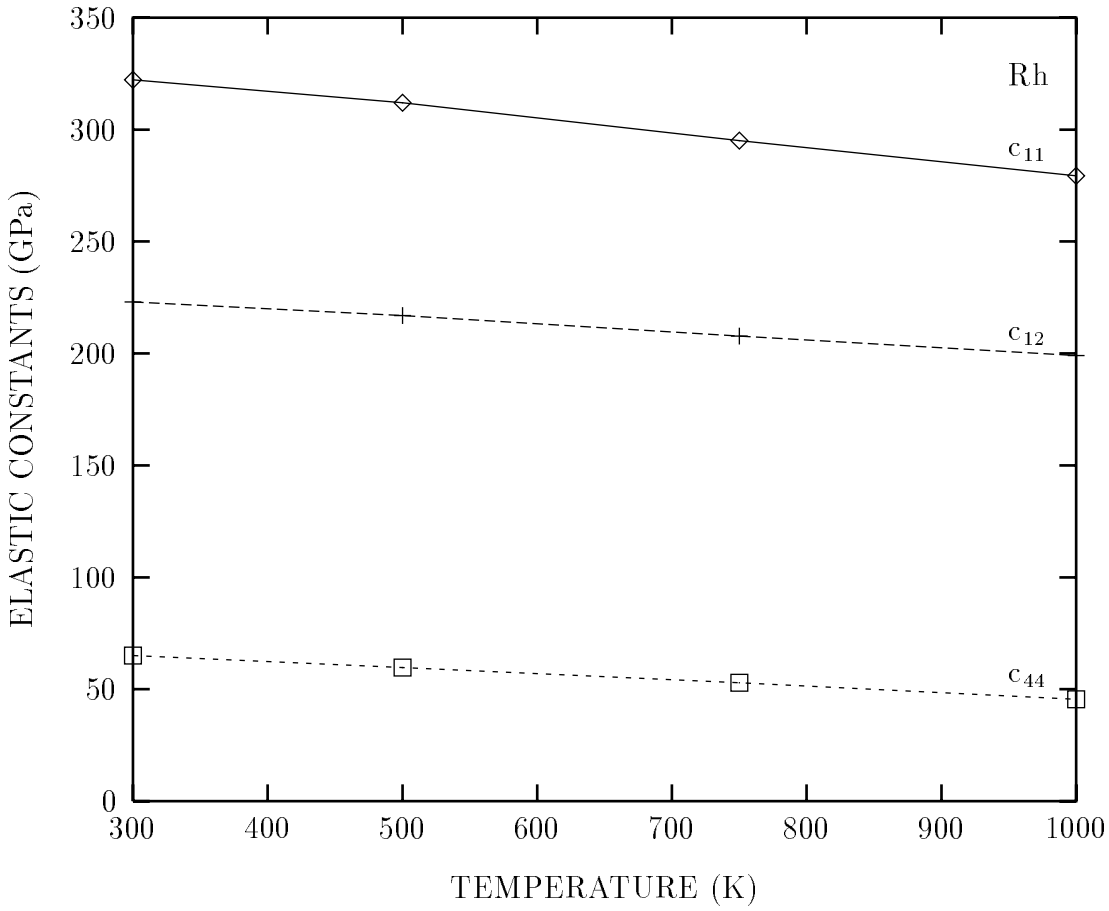

Ni
c_{11}
c_{12}
c_{44}
ELASTIC CONSTANTS (GPa)
TEMPERATURE (K)
220
200
180
160
140
120
100
80
60
40
300
400
500
600
700
800
900
1000

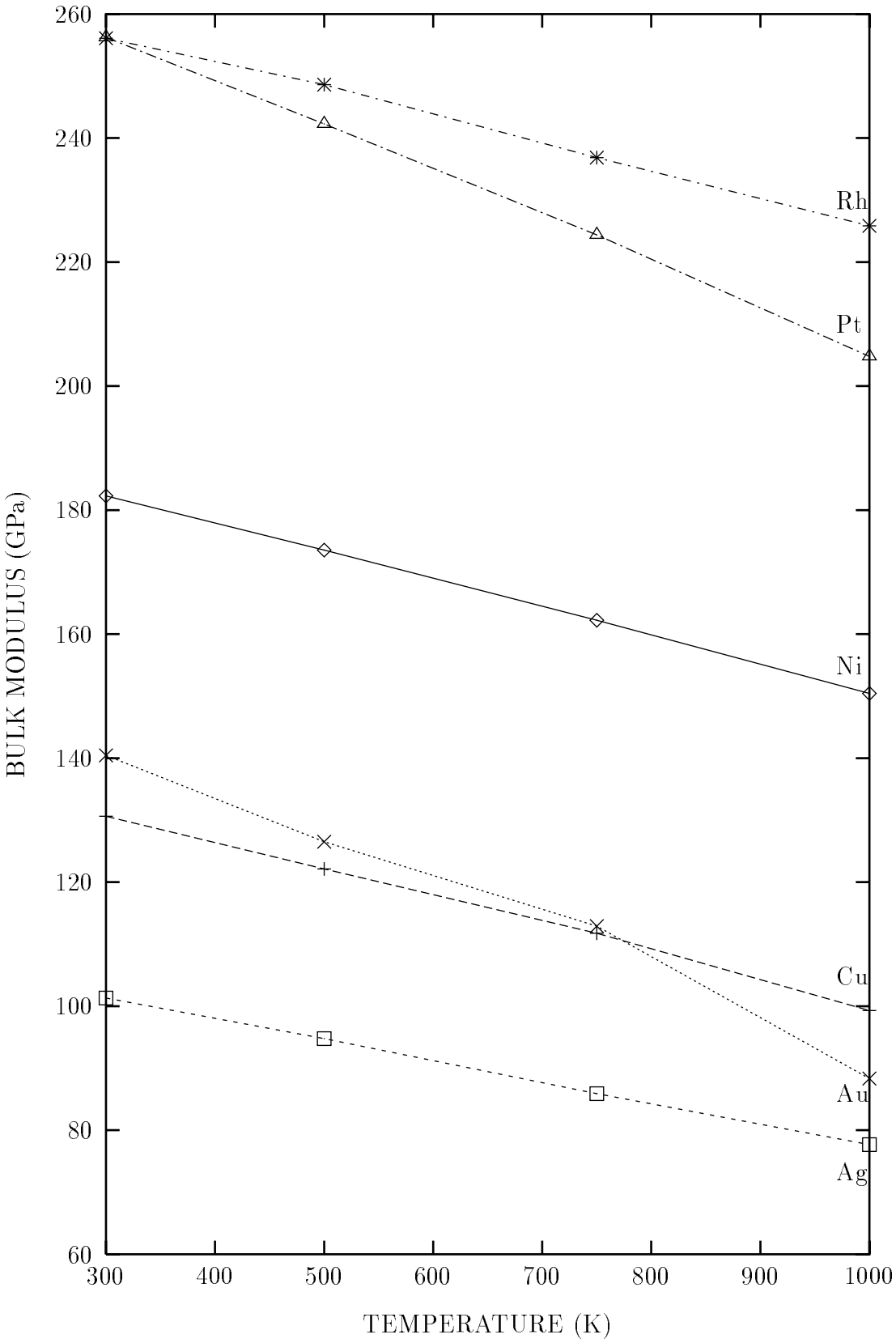

160
140
120
100
80
60
40
20
300
400
500
600
700
800
900
1000
ELASTIC CONSTANTS (GPa)
TEMPERATURE (K)
Cu
c11
c12
c44

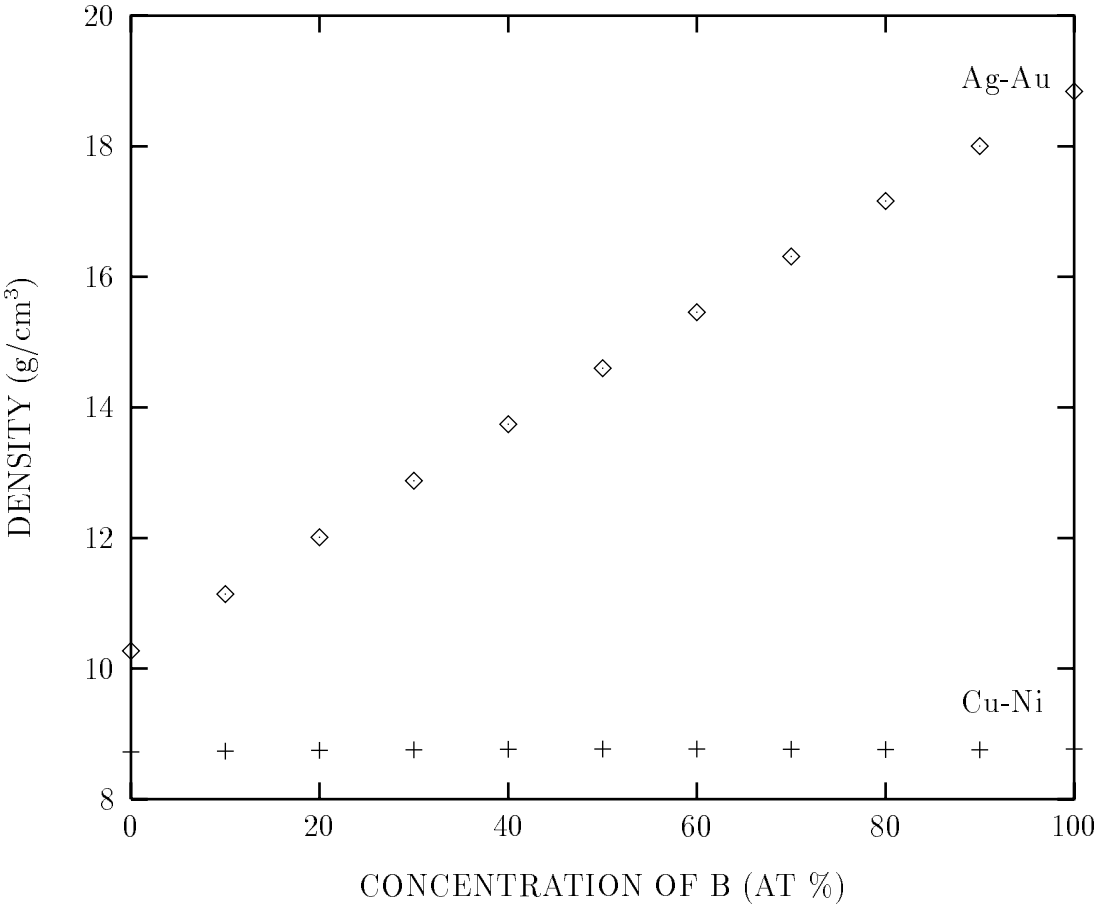

Ag
c_{11}
c_{12}
c_{44}
ELASTIC CONSTANTS (GPa)
TEMPERATURE (K)
130
120
110
100
90
80
70
60
50
40
30
300
400
500
600
700
800
900
1000

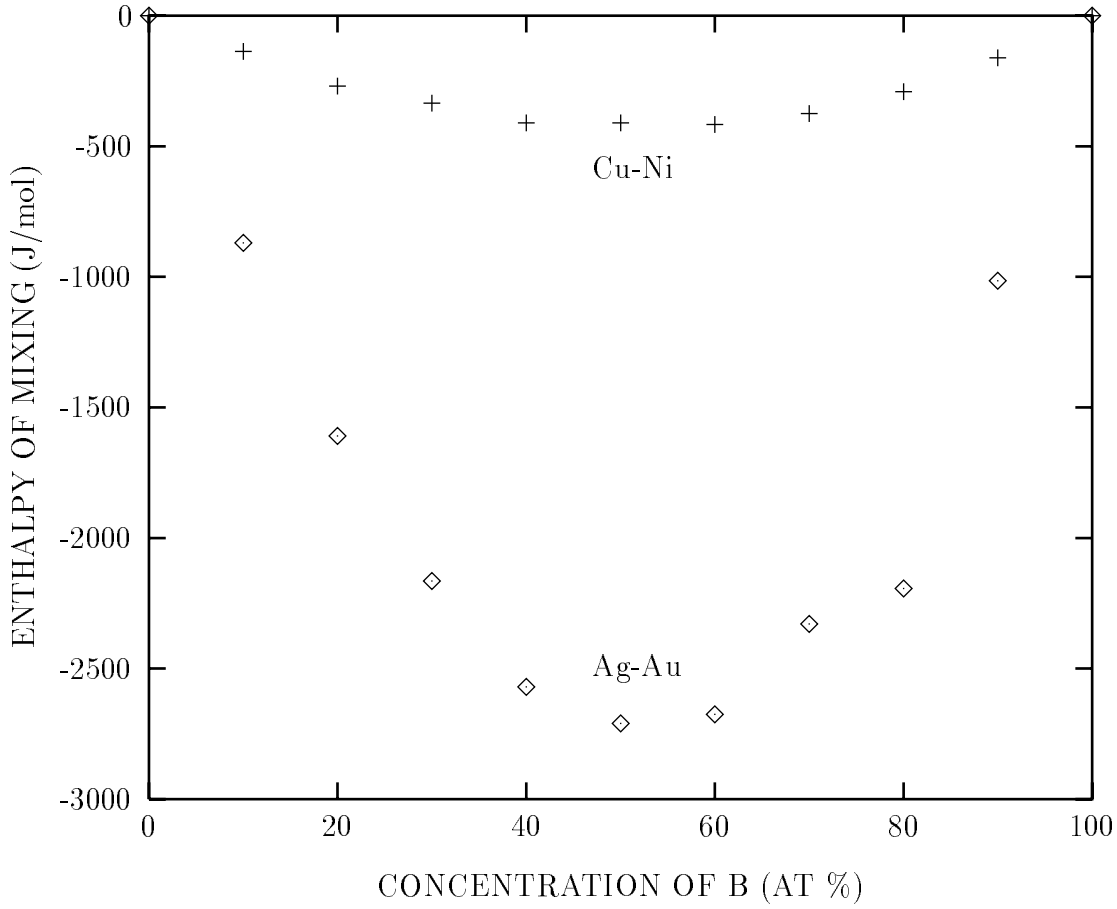

160
140
120
100
80
60
40
20
0
300
400
500
600
700
800
900
1000
ELASTIC CONSTANTS (GPa)
TEMPERATURE (K)
Au
c11
c12
c44


300
250
200
150
100
50
0
300
400
500
600
700
800
900
1000
ELASTIC CONSTANTS (GPa)
TEMPERATURE (K)
Pt
c11
c12
c44


Rh
c_{11}
c_{12}
c_{44}
ELASTIC CONSTANTS (GPa)
TEMPERATURE (K)
350
300
250
200
150
100
50
0
300
400
500
600
700
800
900
1000


260
240
220
200
180
160
140
120
100
80
60
300
400
500
600
700
800
900
1000
BULK MODULUS (GPa)
TEMPERATURE (K)
Rh
Pt
Ni
Cu
Au
Ag


20
18
16
14
12
10
8
0
20
40
60
80
100
DENSITY (g/cm^3)
CONCENTRATION OF B (AT %)
Ag-Au
Cu-Ni


0
-500
-1000
-1500
-2000
-2500
-3000
0
20
40
60
80
100
ENTHALPY OF MIXING (J/mol)
CONCENTRATION OF B (AT %)
Cu-Ni
Ag-Au